

Amendment to the Specification

Please replace paragraph [0060] with the following amended paragraph:

[0060] In other embodiments, the invention can be used to predict BCUT properties (eigenvalues) of combinatorial compounds from BCUT and/or other molecular properties of their respective building blocks. As would be known to a person skilled in the relevant art, a BCUT value is an eigenvalue. As explained by R. S. Pearlman of the University of Texas, College of Pharmacy, the strength of intermolecular interactions depends on atomic charges, atomic polarizabilities, and atomic H-bond-abilities. Thus, Pearlman proposes constructing three classes of matrices to represent compounds: one class with atomic charge-related values on the diagonal, a second class with atomic polarizability-related values on the diagonal, and a third class with H-bond-abilities on the diagonal. Pearlman also proposed using a variety of additional definitions for the off-diagonal elements including functions of interatomic distance, overlaps, computed bond-orders, etc. (See, e.g., R. S. Pearlman, *Novel Software Tools for Addressing Chemical Diversity*, at ~~http://www.netsci.org/Science/Combichem/feature08.html~~ World Wide Web Address: netsci.org/Science/Combichem/feature08.html.) According to Pearlman, the lowest and highest eigenvalues (i.e., BCUT values) of these matrices reflect aspects of molecular structure.